

# Geometric Properties of Quantum Phases

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## Abstract

The Aharonov-Anandan phase is introduced from a physical point of view. Without reference to any dynamical equation, this phase is formulated by defining an appropriate connection on a specific fibre bundle. The holonomy element gives the phase. By introducing another connection, the Pancharatnam phase formula is derived following a different procedure.

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The discovery and subsequent interest in the Berry phase [1] has been relatively recent with respect to the actual period over which quantum mechanics has been in use. Beyond its physical significance, it has generated a great deal of interest into more geometric approaches to quantum mechanics as well as applications of many ideas from the area of differential geometry, in particular, fibre bundles and connections. General relativity and Yang-Mills gauge theories are also examples in which geometrical techniques enter into the study of these theories directly. In fact, quantum mechanics can be looked at geometrically. Here  $\mathcal{H}$  will refer to a Hilbert space in general and any quantum system carries the structure of a Kähler manifold. Even so, the space  $\mathcal{H}$  is not the quantum analog of a classical phase space. In what follows, elements of  $\mathcal{H}$  will be denoted by  $\psi$  or  $|\psi\rangle$ , but the bracket will always appear when the inner product is invoked. The Berry phase is known to depend on the geometric structure of the parameter space itself, so the phase is really a geometric property. The purpose here is to further explore the phase by looking for ways of formulating the ideas in a more intrinsic manner, and to present a different development of the integral formula for the Pancharatnam phase. Simon [2] interpreted this phase as the holonomy of the adiabatic connection in the bundle appropriate to the evolution of the adiabatic eigenstate and expressed it as an integral over a connection one-form. Aharonov and Anandan [3] defined a geometric phase during any cyclic evolution of a quantum system which depends only on the topological features and the curvature of the quantum state space. Wilczek and Zee have considered a nonabelian extension of the phase [4]. Considered in this way, the origin of the geometric phase is due to the parallel transport of a state vector on the curved surface. This is a fundamental notion in modern differential geometry since it is directly related to the concept of a connection, and there are often several ways in which a connection may be defined [5]. Some work which is related to the results here has been done by making use of geodesics [6], a related but different approach from this one.

To see how the idea of a connection can arise physically in this context and to define a connection from a physical point of view, suppose a state vector  $|\psi\rangle$  is an element of a Hilbert space

$\mathcal{H}$  which evolves according to the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \mathbf{H}(t)|\psi(t)\rangle, \quad (1)$$

where  $\mathbf{H}(t)$  is a linear operator, which need not be Hermitian. A new state vector  $|\phi(t)\rangle$  can be defined which has a dynamical phase factor removed. It is given by

$$|\phi(t)\rangle = \exp(i \int_0^t h(\tau) d\tau) |\psi(t)\rangle, \quad (2)$$

such that  $h(t)$  is defined as the real quantity

$$h(t) = \text{Re}\langle\psi(t)|\mathbf{H}(t)|\psi(t)\rangle. \quad (3)$$

Differentiating  $|\phi(t)\rangle$  with respect to  $t$  and requiring that  $|\phi(t)\rangle$  satisfies the Schrödinger equation,

$$i\frac{\partial}{\partial t}|\phi(t)\rangle = -h(t)|\phi(t)\rangle + i \exp(i \int_0^t h(\tau) d\tau) \frac{\partial}{\partial t}|\psi(t)\rangle = -h(t)|\phi(t)\rangle + \mathbf{H}(t)|\phi(t)\rangle.$$

Therefore,  $|\phi(t)\rangle$  satisfies the equation

$$\frac{\partial}{\partial t}|\phi(t)\rangle = i[\mathbf{H}(t) - h(t)]|\phi(t)\rangle. \quad (4)$$

Since  $h(t)$  is the real part of  $\langle\psi|\mathbf{H}|\psi\rangle$ , upon contracting with  $\langle\phi(t)|$ , the right-hand side must be real hence

$$\text{Im} \langle\phi(t)|\frac{\partial}{\partial t}|\phi(t)\rangle = 0. \quad (5)$$

This can be regarded as a parallel transport rule.

To approach this in a more intrinsic manner, the idea of a fibre bundle will be introduced [6]. Any two vectors  $\psi, \phi$  in  $\mathcal{H}$  such that  $\psi = c\phi$  where  $c \in \mathbb{C}$  are physically equivalent since they define the same state and we write  $\psi \sim \phi$ . Thus, the correct phase space of a quantum system is the space of rays in the space  $\mathcal{H}$  and this is denoted by writing  $\mathcal{P}(\mathcal{H}) = \mathcal{H}/\sim$ . The notation  $\sim$  denotes the elements of  $\mathcal{H}$  which differ only by a phase and is referred to as projective Hilbert space here. A canonical projection operator  $\Pi$  can then be defined between these two spaces as

$$\Pi : \mathcal{H} \rightarrow \mathcal{P}(\mathcal{H}), \quad (6)$$

An element of the space  $\mathcal{P}(\mathcal{H})$  may be denoted by  $[\psi] = \Pi(\psi)$ . Thus  $\Pi$  maps  $\psi$  to the ray on which it lies. The fibres  $\Pi^{-1}([\psi])$  are one-dimensional, and this type of vector bundle is referred to as a complex line bundle. The unit sphere is a subset of  $\mathcal{H}$  and is given by

$$S(\mathcal{H}) = \{\psi \in \mathcal{H} | \langle \psi | \psi \rangle = 1\} \subset \mathcal{H}. \quad (7)$$

Thus, we can write equivalently  $\mathcal{P}(\mathcal{H}) = S(\mathcal{H}) / \sim$ . Suppose  $|\phi(s)\rangle$  is a curve in  $\mathcal{H}$  and define

$$|m\rangle = \frac{d}{ds} |\phi(s)\rangle, \quad (8)$$

which denotes the tangent vector to this curve. In terms of  $|\phi(s)\rangle$  and  $|m\rangle$ , we can define

$$A_s = \frac{\text{Im} \langle \phi | m \rangle}{\langle \phi | \phi \rangle}. \quad (9)$$

A transformation acting on  $|\phi(s)\rangle$  which has the form  $|\phi(s)\rangle \rightarrow |\hat{\phi}(s)\rangle = \exp(i\alpha(s))|\phi(s)\rangle$  has the structure of a gauge transformation. Differentiating the transformed  $|\phi(s)\rangle$ , with respect to  $s$  gives

$$|\hat{m}\rangle = e^{i\alpha} \frac{d}{ds} |\phi(s)\rangle + i \frac{d\alpha}{ds} e^{i\alpha} |\phi(s)\rangle. \quad (10)$$

From (10), the transformed function  $\hat{A}_s$  can be obtained in the form

$$\hat{A}_s = \frac{\text{Im} \langle \hat{\phi} | \hat{m} \rangle}{\langle \hat{\phi} | \hat{\phi} \rangle} = A_s + i \frac{d\alpha}{ds}. \quad (11)$$

Therefore,  $A_s$  which is defined by expression (9) transforms like the vector potential in electrodynamics. The parallel transport law (5) then states that  $A_s$  vanishes along the actual curve  $|\phi(s)\rangle$  which is taken by the quantum system in the quantum space.

Let  $|\psi(t)\rangle$  be a solution of the Schrödinger equation which is cyclic. This means that it returns to the initial ray after a given time  $\tau$  and as well specifies a curve in  $\mathcal{H}$ . Under the map  $\Pi$  this curve is mapped to a closed curve in  $\mathcal{P}(\mathcal{H})$ . Given a closed curve  $\sigma(s)$  in  $\mathcal{P}(\mathcal{H})$ , let us consider the curve in  $\mathcal{H}$ , which is traced out by the state vector  $|\phi(s)\rangle$ . Using the parallel transport law, the curve is determined by the condition that  $A_s = 0$  holds along the actual curve. Define the integral

$$\gamma = \oint_{\Gamma} A_s ds. \quad (12)$$

The path  $\Gamma$  in (12) is traced out along the curve  $|\phi(s)\rangle$  in the space  $\mathcal{H}$  which has been made closed by the vertical curve joining  $|\phi(\tau)\rangle$  to  $|\phi(0)\rangle$ . The segment along  $|\phi(s)\rangle$  generates the actual evolution of the system, but by the parallel transport law (5), it is clear that  $A_s = 0$  along this segment. It is left to the vertical segment of the trajectory to contribute the phase difference between the states  $|\phi(0)\rangle$  and  $|\phi(\tau)\rangle$ . The integral in (12) is gauge invariant on account of the transformation rule (11), and it can therefore be considered an integral on  $\mathcal{P}(\mathcal{H})$ . By Stokes theorem,  $\gamma$  can also be expressed in the form

$$\gamma = \int_S dA_s = \int_S F, \quad (13)$$

such that  $S$  is any surface in  $\mathcal{P}(\mathcal{H})$  bounded by the closed curve  $\sigma(s)$  in  $\mathcal{P}(\mathcal{H})$ . The field strength  $F$  which appears in (13) is a gauge invariant two-form as well. From this, it can be seen that  $\gamma$  in (12) and (13) is a geometrical quantity depending on the geometric curve  $\sigma(s)$ . This is the version of Berry's phase in a cyclic evolution of the quantum system.

Let us formulate this in a more geometric way by looking for an appropriate connection in a principle  $U(1)$ -bundle,  $S(\mathcal{H}) \rightarrow \mathcal{P}(\mathcal{H})$ . To introduce a connection we have to define a subspace of horizontal vectors. Identifying the tangent space  $T_\psi S(\mathcal{H})$  as a linear subspace in  $\mathcal{H}$ , a decomposition exists of the form

$$T_\psi S(\mathcal{H}) = V_\psi + H_\psi. \quad (14)$$

Hence the subspaces of vertical and horizontal vectors are linear subspaces of  $\mathcal{H}$ . A fibre  $\Pi^{-1}(\psi)$  consists of all vectors of the form  $e^{i\lambda}\psi$ . The vertical subspace  $V_\psi$  in (14) can then be defined by

$$V_\psi = \{i\lambda\psi \mid \lambda \in \mathbb{R}\},$$

which can be identified with  $u(1)$ . To define a natural connection, let  $X$  be a vector tangent to  $S(\mathcal{H})$  at  $\psi$ . Then  $X$  is called a horizontal vector with respect to a natural connection if

$$\langle \psi | X \rangle = 0.$$

The set of horizontal vectors at  $\psi$  in (14) can be defined as follows

$$H_\psi = \{X \in \mathcal{H} \mid \langle \psi | X \rangle = 0\}.$$

A curve  $t \rightarrow \psi(t) \in S(\mathcal{H})$  is horizontal if

$$\langle \psi(t) | \dot{\psi}(t) \rangle = 0.$$

Since  $\langle \psi | \psi \rangle = 1$ , differentiating with respect to the parameter,  $\langle \dot{\psi} | \psi \rangle + \langle \psi | \dot{\psi} \rangle = 0$  which implies that  $Re \langle \psi(t) | \dot{\psi}(t) \rangle = 0$  and so the horizontal condition can be expressed as

$$Im \langle \psi(t) | \dot{\psi}(t) \rangle = 0.$$

A connection one-form  $\mathcal{A}$  in a principal  $U(1)$  bundle  $S(\mathcal{H}) \rightarrow \mathcal{P}(\mathcal{H})$  is a  $u(1)$ -valued one-form on  $S(\mathcal{H})$ . Take an element  $X \in S(\mathcal{H}) \subset \mathcal{H}$  and define in  $u(1)$

$$A_\psi(X) = i Im \langle \psi | X \rangle.$$

Therefore,  $X$  is horizontal at a point  $\psi \in S(\mathcal{H})$  if  $A_\psi(X) = 0$ . Consider now a local connection form  $A$  on  $\mathcal{P}(\mathcal{H})$  such that  $\Psi : \mathcal{P}(\mathcal{H}) \rightarrow S(\mathcal{H})$  is a local section. The pull back of  $\mathcal{A}$

$$A = i\Psi^*\mathcal{A},$$

defines a local connection one-form on  $\mathcal{P}(\mathcal{H})$ . This implies the local connection  $A$  in gauge  $\psi$  can be written

$$A = i\langle \psi | d\psi \rangle. \tag{16}$$

Once the connection has been defined as in (16), the corresponding holonomy element may be computed from  $A$  as

$$\Phi(C) = \exp(i \oint_C A), \tag{17}$$

where  $C$  is a closed curve in  $\mathcal{P}(\mathcal{H})$ .

Some additional information will be needed to show the remaining result. Take two nonorthogonal vectors  $\psi_1, \psi_2 \in S(\mathcal{H})$ . The phase of their scalar product will be called the *relative* phase or phase difference between  $\psi_1$  and  $\psi_2$ . Thus  $\langle \psi_1 | \psi_2 \rangle = re^{i\alpha_{12}}$  so  $\alpha_{12}$  is the phase difference between  $\psi_1$  and  $\psi_2$ . Hence  $\psi_1$  and  $\psi_2$  are in phase or parallel if  $\langle \psi_1 | \psi_2 \rangle$  is real and positive. There is a relation then between any two nonorthogonal vectors  $\psi \sim \phi$  if and only if they are in phase. This

procedure is yet another way of equipping a principal  $U(1)$  fibre bundle  $S(\mathcal{H}) \rightarrow \mathcal{P}(\mathcal{H})$  with a connection.

Furthermore, if  $p_1$  and  $p_2$  are two points in  $\mathcal{P}(\mathcal{H})$ , then let  $\psi_1$  and  $\psi_2$  be two arbitrary nonorthogonal state vectors in  $S(\mathcal{H})$  projecting down to  $p_1$  and  $p_2$ , respectively. A real plane in  $\mathcal{H}$  can be defined by the pair  $\psi_1$  and  $\psi_2$  in the following way  $\{\psi = \xi_1\psi_1 + \xi_2\psi_2 | \xi_1, \xi_2 \in \mathbb{R}\} \subset \mathcal{H}$ . This gives a natural way to obtain a geodesic since the intersection of any real plane with the unit sphere  $S(\mathcal{H})$  is a great circle. This defines a geodesic on  $S(\mathcal{H})$  with respect to the metric induced from  $\mathcal{H}$ . A geodesic on the sphere  $S(\mathcal{H})$  projects to a geodesic on  $\mathcal{P}(\mathcal{H})$ , and hence each geodesic on  $\mathcal{P}(\mathcal{H})$  is a closed curve since it is the projection of a closed curve. Thus, a geodesic joining  $\psi_1$  and  $\psi_2$  on  $S(\mathcal{H})$  is an arc of a great circle passing through  $\psi_1$  and  $\psi_2$  and is parametrized by an angle  $\theta \in [0, 2\pi)$  such that

$$\psi(\theta) = \xi_1(\theta)\psi_1 + \xi_2(\theta)\psi_2. \quad (18)$$

Now define the real parameter  $a = \text{Re} \langle \psi_1 | \psi_2 \rangle$  and suppose that  $a > 0$ . The normalization condition  $\langle \psi(\theta) | \psi(\theta) \rangle = 1$  takes the form

$$\xi_1^2 + 2a\xi_1\xi_2 + \xi_2^2 - 1 = 0. \quad (19)$$

In terms of the angle  $\theta$ , the coefficients  $\xi_1$  and  $\xi_2$  can be written as

$$\xi_1(\theta) = \cos \theta - \frac{a}{\sqrt{1-a^2}} \sin \theta, \quad \xi_2(\theta) = \frac{1}{\sqrt{1-a^2}} \sin \theta, \quad (20)$$

which satisfy (19). Moreover,  $\psi(0) = \psi_1$  and  $\psi(\theta_0) = \psi_2$ , where the angle  $\theta_0$  is defined by  $\cos \theta_0 = a$  such that  $\theta_0 \in [0, \pi/2)$ .

It is remarkable that the Pancharatnam phase can be expressed as a line integral of  $A_s$  with the use of the geodesic rule. Let  $|\phi_1\rangle$  and  $|\phi_2\rangle$  be any two nonorthogonal states in  $\mathcal{H}$  with phase difference  $\beta$ . Let  $|\phi(s)\rangle$  be any geodesic curve connecting  $|\phi_1\rangle$  to  $|\phi_2\rangle$  so that  $|\phi(0)\rangle = |\phi_1\rangle$  and  $|\phi(1)\rangle = |\phi_2\rangle$ . Then the phase difference  $\beta$  is given by

$$\beta = \int A_s ds, \quad (21)$$

where  $A_s$  is given by the natural connection (9).

Consider two points  $p_1, p_2 \in \mathcal{P}(\mathcal{H})$ , and let  $\sigma$  be the shorter arc of the geodesic which connects  $p_1$  and  $p_2$ . Suppose  $\tilde{\sigma} : t \rightarrow \psi(t) \in S(\mathcal{H})$  is a horizontal lift of  $\sigma$  with respect to the natural connection in the principal fibre bundle  $S(\mathcal{H}) \rightarrow \mathcal{P}(\mathcal{H})$ . Then a parallel transport of  $\psi$  keeps  $\psi(t)$  in phase with  $\psi(0)$ . To see this, let  $C$  be a geodesic in  $S(\mathcal{H})$  projecting to  $\sigma$  in  $\mathcal{P}(\mathcal{H})$ . Any geodesic on the unit sphere  $S(\mathcal{H})$  is uniquely defined by a real plane in  $\mathcal{H}$  spanned by two vectors  $\psi_1$  and  $\psi_2$ . The shorter arc of the closed geodesic can be written as in (18) and is a horizontal lift of  $\sigma$  if and only if  $\langle \psi_1 | \psi_2 \rangle$  is real and positive. Thus,  $\psi_1$  and  $\psi_2$  are in phase. Using (18), we can work out  $\langle \psi(\theta_1) | \psi(\theta_2) \rangle$  with  $\langle \psi_1 | \psi_2 \rangle = a$  and this is

$$\begin{aligned} \langle \psi(\theta_1) | \psi(\theta_2) \rangle &= \xi_1(\theta_1) \xi_1(\theta_2) + \xi_2(\theta_1) \xi_1(\theta_2) \langle \psi_2 | \psi_1 \rangle + \xi_1(\theta_1) \xi_2(\theta_2) \langle \psi_1 | \psi_2 \rangle + \xi_2(\theta_1) \xi_2(\theta_2) \\ &= \cos \theta_1 \cos \theta_2 + \frac{a^2}{1-a^2} \sin \theta_1 \sin \theta_2 + \frac{1}{1-a^2} \sin \theta_1 \sin \theta_2 \\ &\quad - \frac{a^2}{1-a^2} \sin \theta_1 \sin \theta_2 - \frac{a^2}{1-a^2} \sin \theta_1 \sin \theta_2 \\ &= \cos(\theta_1 - \theta_2) > 0, \end{aligned}$$

since  $\theta_1, \theta_2 \in [0, \theta_0]$  and  $\theta_0$  is given by solving  $\cos \theta_0 = a$ . Therefore, any two points belonging to the horizontal lift  $\tilde{\sigma}$  are in phase.

To finish the proof of (21), carry out a gauge transformation  $|\phi(s)\rangle = \exp(i\alpha(s))|\tilde{\phi}(s)\rangle$  of the horizontal lift  $|\tilde{\phi}(s)\rangle$  of the geodesic in  $\mathcal{P}$ . where  $\alpha(s)$  is chosen such that  $\alpha(0) = 0$  and  $\alpha(1) = \beta$ . Then  $|\phi(s)\rangle$  remains a geodesic curve, since the geodesic equation is gauge covariant and connects  $|\phi_1\rangle$  to  $|\phi_2\rangle$ . Thus since  $\tilde{A}_s$  is zero on the horizontal curve, the right-hand side of (21) can be integrated to give

$$\int_0^1 \frac{d\alpha(s)}{ds} ds = \alpha(1) - \alpha(0) = \beta.$$

This completes the proof.



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